4. Semi-Classical Theory of Atomic Collision Based on the Dynamical Representation and Its Application to (Li-Na)^+ System

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to reproduce the symmetric spectrum. This model is considered to be reasonable for the structurally disordered system. The knowldge of the local asymmetries of ligand field is expected to provide the information concerning with the angular distribution of the atomic arrangement, which can be scarcely obtained by other techniques.

The temperature dependence of hyperfine field of the amorphous oxide Fe_2O_3-BaO-B_2O_3 was examined accurately. The hyperfine field decreases slower than the corresponding Brillouin function with increasing temperature. This result is quite different from that of most of the amorphous alloys. The reason for the difference remains still unsettled.

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ABSTRACT

In the theoretical treatment of atom-atom or ion-atom collision processes the adiabatic state representation is generally the best one unless collision energies are very high. In this representation the electronic transitions can be interpreted in terms of non-adiabatic coupling terms. There are two kinds of non-adiabatic couplings, i.e., radial coupling and rotational coupling. The non-adiabatic radial coupling which governs a transition between the adiabatic molecular states of the same symmetry has been investigated successfully. The transition occurs locally at avoided crossing of potential energy curves. The Landau-Zener-Stueckelbelg theory, and its extentions and modifications can be successfully applied to the problem. Rotational coupling presents another important non-adiabatic coupling which governs a transition between the adiabatic states of different symmetry. Because of the difficulty in the analytical structure of this coupling, any good analytical theory to deal with the rotationally induced non-adiabatic transitions has not been yet developed.

Recently the semiclassical theory of rotationally induced non-adiabatic transitions is proposed based on a "dynamical state" representation. In this new representation all transitions can be considered to occur locally at the avoided crossings of the new dynamical effective potential curves. Because of this localized behavior, we can deal with a many-state

collision problem step-by-step based on the two-state collision theory.

In this paper we have applied this theory to the follwing collision processes:

$$Li^+ + Na\,(3s) \longrightarrow Li^*\,(2p) + Na^+$$
$$\longrightarrow Li\,(2s) + Na^+$$

Three lowest electronic states (two Σ states and one Π state) of the $(Li\text{-}Na)^+$ system are involved in these collision processes. There are one radial coupling between the two Σ states (an avoided a crossing at about 14.8 a.u. of internuclear distance), and one rotational coupling between the second Σ and the Π states (a real crossing at about 5.7 a.u.). Purposes of this work are (1) to investigate the usefulness of the semiclassical theory by applying it to these actual collision problems, and (2) to try to explain the experimental results by the purely theoretical analysis.

First we have calculated the transition probabilities for the two-state problems semiclassically and quantum mechanically in order to investigate the validity of the semiclassical theory. Agreement between them is found to be very good, indicating the usefulness of our semiclassical theory. Second we have derived the expressions of the deflection functions, differential cross sections, and total cross sections for the realistic three-state $(Li\text{-}Na)^+$ system by the new semiclassical theory. Third the numerical calculations of these quantities have been performed and compared with experiments.